Process Systems Engineering

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Exercise 1

Material balance HDA plant

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Conceptual design

- It is a systematic procedure to evaluate different plant alternatives on an economic basis
- In theory, the alternatives can be of the order of 10^4 - 10^9
- Missing elements: environmental considerations, safety, controllability, ease of start-up and shutdown,…

Conceptual design (2)

Steps:

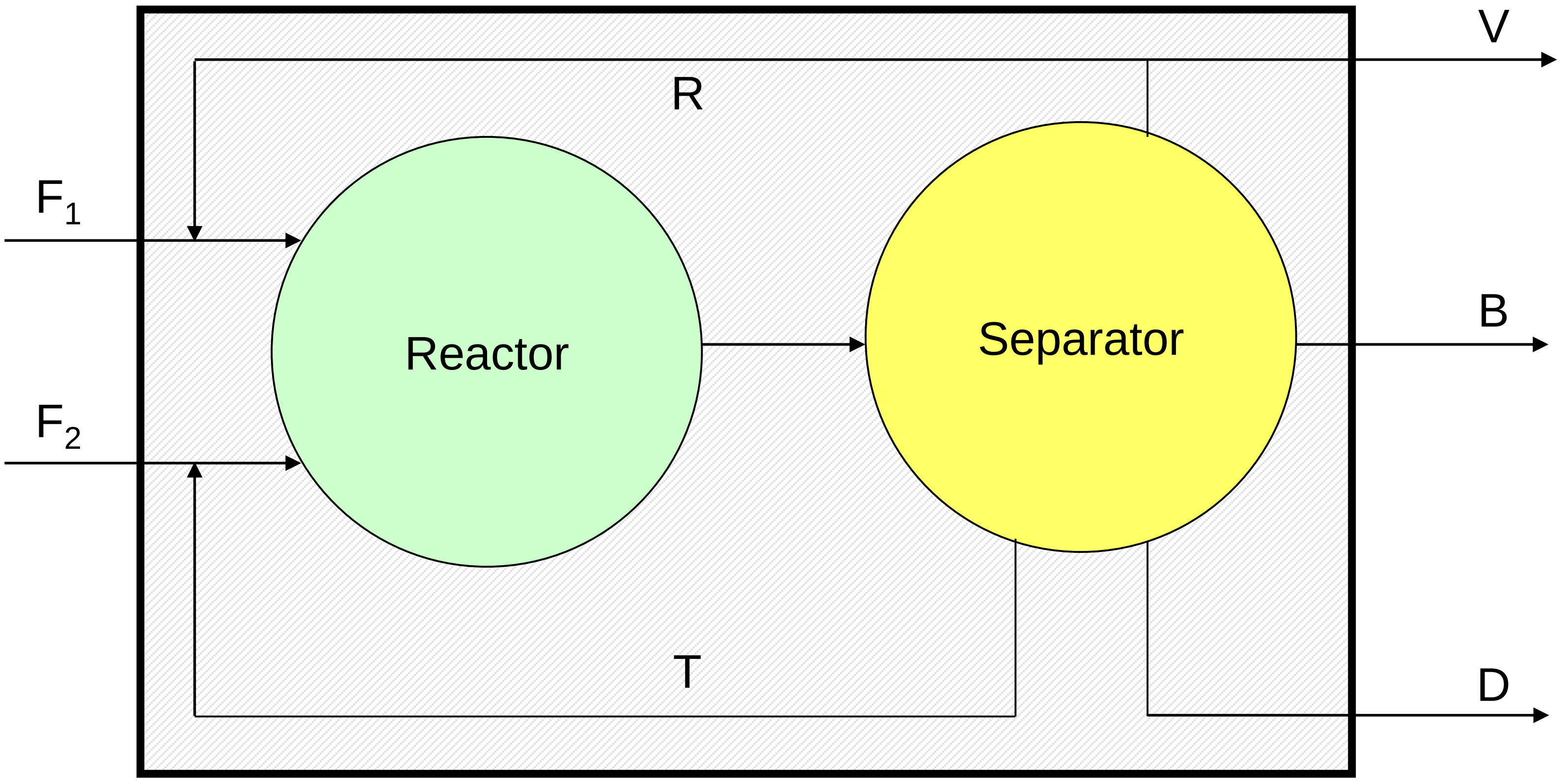
1. Selecting the type of process
2. Identification of the input-output structure (EP2)
3. Identification of recycling (EP3)
4. Design of the separator section(EP4)
5. Thermal integration process (EP5)

Increased detail from the first to the last point

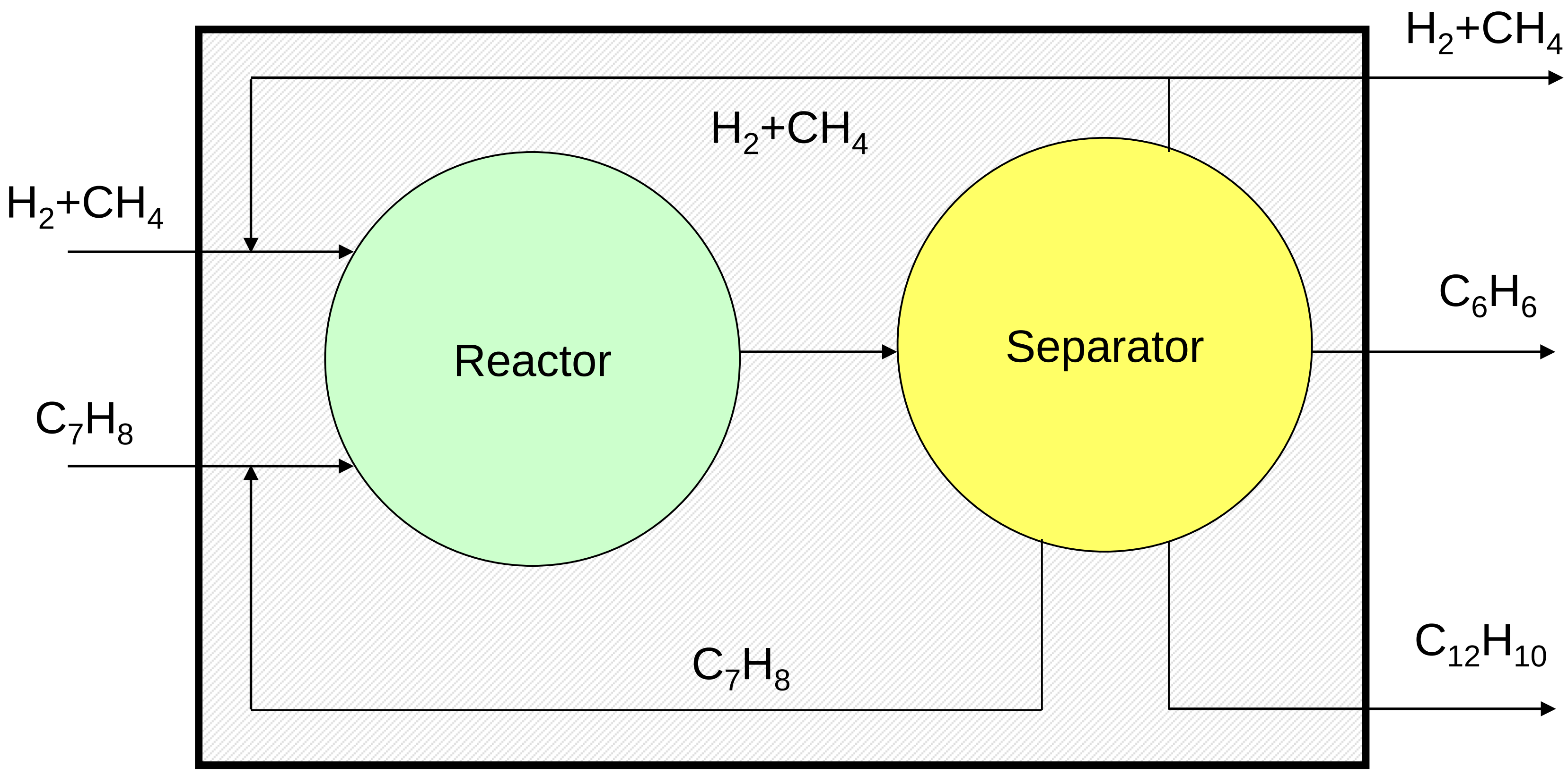
Introduction

The exercises of the Process Systems Engineering course deal with the basic design and economic analysis of the Hydrodealkylation (HDA) process of toluene to give benzene.

HDA process



HDA process



Reactions

Desired reaction

$$C_7H_8 + H_2 \rightarrow C_6H_6 + CH_4$$

Side reaction

$$2C_6H_6 \rightarrow C_{12}H_{10} + H_2$$

Degrees of freedom

Selection of reactor

Presence of recycle?

- Recycling of toluene and unreacted hydrogen

Presence of drains?

- Purging part of the gas stream to prevent the accumulation of methane in the system

Degrees of freedom

- Choice of reactor
  - Conditions of input currents
  - Residence time or volume of the reactor
  - Operating conditions (pressure and temperature)

Degrees of freedom

Conditions of input streams

- The current of fresh hydrogen contains 5% mol of methane
- The reagents are at room temperature
- The ratio between hydrogen and toluene in the inlet of the reactor must be, on the one hand high to avoid coking and on the other hand low to reduce recycling costs. It is suggested to use a ratio equal to 5

Residence time and reactor volume

Determined by the following specifics

- The selectivity must be $\geq$ 96%
- The productivity of benzene must be = 265 kmol/h
- The purity of benzene must be $\geq$ 0.9997

Degrees of freedom

Operating conditions

Operating Pressure

PROS: increasing the pressure there is an increase of products concentration due to increased reaction speed.
CONS: pressure increase rises compression costs

$\Rightarrow$ Reactor operative pressure: P = 34 bar

Degrees of freedom

Operating conditions

Operating Temperature

The contribution of any catalyst is not necessary (simplified assumption).

- The main reaction is exothermic
- The side reaction becomes more important at high temperature (higher activation energy)

⇒ we should find a compromise between main and side reactions kinetic rates.

Range of economic interest : 600 – 750 °C
(Carry out tests every 50 °C)

Degrees of freedom

Selection of the reactor

The product of interest is an intermediate in the reaction scheme:

Toluene ⇒ Benzene ⇒ Biphenyl

⇓

Necessary to control contact time (while maintaining the selectivity above 96%)

⇓

Must use a PFR reactor type!

Simplifying assumptions

- The short-cut assumptions for the separation section allow considering:

$\Rightarrow V = H_2 + CH_4$

$\Rightarrow R = H_2 + CH_4$

$\Rightarrow B = C_6H_6$

$\Rightarrow T = C_7H_8$

$\Rightarrow D = C_{12}H_{10}$

Currents/Compositions Matrix

	H_2	CH_4	C_6H_6	C_7H_8	$C_{12}H_{10}$
F_1	0.95	0.05	0	0	0
F_2	0	0	0	1	0
B	0	0	1	0	0
D	0	0	0	0	1
V	x_V	$1- x_V$	0	0	0
R	x_V	$1- x_V$	0	0	0
T	0	0	0	1	0

Definitions

- Selectivity: $$\sigma = \frac{\text{Desired moles of Product}}{\text{Moles converted}} = \frac{n_{C_6H_6}}{n_{C_7H_8}^{ini} - n_{C_7H_8}^{fin}}$$

- Conversion: $$\xi = \frac{\text{Reacted Moles}}{\text{Initial moles}} = \frac{n_{C_7H_8}^{ini} - n_{C_7H_8}^{fin}}{n_{C_7H_8}^{ini}} = 1 - \frac{n_{C_7H_8}^{fin}}{n_{C_7H_8}^{ini}}$$

- Residence Time: $$\tau = \frac{\text{Reactor volume}}{\text{Volumetric flow rate}}$$

Requirements

1. Select the type of process: batch or continuous?

2. Write global material balances, given the reaction stoichiometry. It should be possible to give an estimate of the incoming, outgoing and recycle flowrates

3. Identify the degrees of freedom of the system

4. Determine the influence of operating variables on the plant management

Unknowns determination

- 7 flows (F_1, F_2, B, D, V, R, T)
- 1 composition (x_v) or splitting ratio R/(R+V)
- Conversion (R1 and R2)
- Operating temperature

Specifications

We have the following specifications:

- Selectivity
- Productivity
- Hydrogen / toluene ratio at reactor inlet (recycles must be considered)

We need to define degrees of freedom